## (Primitive) Mathematical Model of Neuron



## Formal neuron

- $x_{1}, \ldots, x_{n}$ real inputs



## Formal neuron



## Formal neuron



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## Formal Neuron vs Linear Models

- If $\sigma$ is a linear threshold function

$$
\sigma(\xi)= \begin{cases}1 & \xi \geq 0 \\ 0 & \xi<0\end{cases}
$$

we obtain a linear classifier.

- If $\sigma$ is identity, i.e., $\sigma(\xi)=\xi$, we obtain a linear (affine) function.
- If $\sigma(\xi)=1 /\left(1+e^{-\xi}\right)$ we obtain the logistic regression.

Also, other activation functions are used in neural networks!

## Activation Functions

Sigmoid
$\sigma(x)=\frac{1}{1+e^{-x}}$


## Leaky ReLU $\max (0.1 x, x)$


tanh
$\tanh (x)$


ReLU
$\max (0, x)$

ELU

$$
\begin{cases}x & x \geq 0 \\ \alpha\left(e^{x}-1\right) & x<0\end{cases}
$$



## Multilayer Perceptron (MLP)



- Neurons are organized in layers (input layer, output layer, possibly several hidden layers)
- Layers are numbered from 0 ; the input is 0 -th
- Neurons in the $\ell$-th layer are connected with all neurons in the $\ell+1$-th layer


## Multilayer Perceptron (MLP)

Output

Hidden

Input


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Intuition: The network computes a function as follows: Assign input values to the input neurons and 0 to the rest. Proceed upwards through the layers, one layer per step. In the $\ell$-th step consider output values of neurons in $\ell-1$-th layer as inputs to neurons of the $\ell$-th layer. Compute output values of neurons in the $\ell$-th layer.

## Example



- Activation function: linear threshold

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## Classical Example - ALVINN



## A Bit of History

- Perceptron (Rosenblatt et al, 1957)
- Single layer (i.e. no hidden layers), the activation function linear threshold
(i.e., a bit more general linear classifier)
- Perceptron learning algorithm
- Used to recognize digits


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- Perceptron learning algorithm
- Used to recognize digits
- Adaline (Widrow \& Hof, 1960)
- Single layer, the activation function identity (i.e., a bit more linear function)
- Online version of the gradient descent
- Used a new circuitry element called memristor which was able to "remember" history of current in form of resistance

In both cases, the expressive power is rather limited - can express only linear decision boundaries and linear (affine) functions.

## A Bit of History

One of the famous (counter)-examples: XOR


No perceptron can distinguish between ones and zeros.

## XOR vs Multilayer Perceptron


(Here $\sigma$ is a linear threshold function.)

$$
P_{1}:-1+2 x_{1}+2 x_{2}=0 \quad P_{2}: 3-2 x_{1}-2 x_{2}=0
$$

The output neuron performs an intersection of half-spaces.

## Boolean functions

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- The second layer may, e.g., make intersections of the half-spaces $\Rightarrow$ convex sets.
- The third layer may, e.g., make unions of some convex sets.


## Example

Consider a triangle $T$ in $\mathbb{R}^{2}$ determined by three vertices $(-1,-1),(1,-1),(-1,2)$.
Give an example of a multi-layer perceptron (MLP) with two input neurons and a single output neuron computing the function $F: \mathbb{R}^{2} \rightarrow\{0,1\}$ defined as follows:
$F\left(x_{1}, x_{2}\right)=1$ iff $\left(x_{1}, x_{2}\right)$ lies either inside, or on the border of $T$ All activation functions in the network should be

$$
\sigma(\xi)=\operatorname{sgn}(\xi)= \begin{cases}1 & \xi \geq 0 ; \\ 0 & \xi<0 .\end{cases}
$$

Homework: Consider $F\left(x_{1}, x_{2}\right)=1$ iff $\left(x_{1}, x_{2}\right)$ lies inside of $T$ (but not on the border)









AND

## Expressive Power of MLP

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But for a long time, at least throughout 60 s and 70 s, nobody well-known knew any efficient method for training multilayer networks!
... then an efficient way of using the gradient descent was published in 1986 !

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y_{j}=\sigma_{j}\left(\xi_{j}\right)
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Here $\sigma_{j}$ is an activation function of the neuron $j$.
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- Fixing weights of all neurons, the network computes a function $F[\vec{w}]: \mathbb{R}^{|X|} \rightarrow \mathbb{R}^{|Y|}$ as follows: Assign values of a given vector $\vec{x} \in \mathbb{R}^{|X|}$ to the input neurons, evaluate the network, then $F[\vec{w}](\vec{x})$ is the vector of values of the output neurons.
Here we implicitly assume a fixed orderings on input and output vectors.


## MLP - Learning

- Given a set $D$ of training examples:

$$
D=\left\{\left(\vec{x}_{k}, \vec{d}_{k}\right) \quad \mid \quad k=1, \ldots, p\right\}
$$

Here $\vec{x}_{k} \in \mathbb{R}^{|X|}$ and $\vec{d}_{k} \in \mathbb{R}^{|Y|}$. We write $d_{k j}$ to denote the value in $\vec{d}_{k}$ corresponding to the output neuron $j$.

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- Error Function: $E(\vec{w})$ where $\vec{w}$ is a vector of all weights in the network. The choice of $E$ depends on the solved task (classification vs regression etc.). Example (Squared error):

$$
E(\vec{w})=\sum_{k=1}^{p} E_{k}(\vec{w})
$$

where

$$
E_{k}(\vec{w})=\frac{1}{2} \sum_{j \in Y}\left(y_{j}[\vec{w}]\left(\vec{x}_{k}\right)-d_{k j}\right)^{2}
$$

## MLP - Batch Gradient Descent

The algorithm computes a sequence of weights $\vec{w}^{(0)}, \vec{w}^{(1)}, \ldots$.

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$$
\Delta w_{j i}^{(t)}=-\varepsilon(t) \cdot \frac{\partial E}{\partial w_{j i}}\left(\vec{w}^{(t)}\right)
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Note that $\frac{\partial E}{\partial w_{j i}}\left(\vec{w}^{(t)}\right)$ is a component of $\nabla E$, i.e., the weight change in the step $t+1$ can be written as follows: $\vec{w}^{(t+1)}=\vec{w}^{(t)}-\varepsilon(t) \cdot \nabla E\left(\vec{w}^{(t)}\right)$.

## Illustration of Gradient Descent - XOR



Source: Pattern Classification (2nd Edition); Richard O. Duda, Peter E. Hart, David G. Stork

## Stochastic Gradient Descent (SGD)

Assume that $E(\vec{w})=\sum_{k=1}^{p} E_{k}(\vec{w})$ where $E_{k}(\vec{w})$ is an error w.r.t. the single training example $\left(\vec{x}_{k}, \vec{d}_{k}\right)$.

- weights in $\vec{w}^{(0)}$ are randomly initialized to values close to 0
- in the step $t+1$ (here $t=0,1,2 \ldots$ ), weights $\vec{w}^{(t+1)}$ are computed as follows:
- Choose (randomly) a set of training examples $T \subseteq\{1, \ldots, p\}$
- Compute

$$
\vec{w}^{(t+1)}=\vec{w}^{(t)}+\Delta \vec{w}^{(t)}
$$

where

$$
\Delta \vec{w}^{(t)}=-\varepsilon(t) \cdot \sum_{k \in T} \nabla E_{k}\left(\vec{w}^{(t)}\right)
$$

- $0<\varepsilon(t) \leq 1$ is a learning rate in step $t+1$
- $\nabla E_{k}\left(\vec{w}^{(t)}\right)$ is the gradient of the error of the example $k$

Note that the random choice of the minibatch is typically implemented by randomly shuffling all data and then choosing minibatches sequentially.

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- In practice, does converge to low error for many large networks on (big) real data.
- Many epochs (thousands) may be required, hours or days of training for large networks.

There are many issues concerning learning efficiency (data normalization, selection of activation functions, weight initialization, learning rate, efficiency of the gradient descent itself etc.) - see PV021.

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- Keep a hold-out validation set and test the error of the network on this set after every epoch. Stop training when additional epochs actually increase the validation error.
The validation error can be measured by completely different means than the training error $E$.


## Hidden Neurons Representations

Trained hidden neurons can be seen as newly constructed features.
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Consider a two-layer MLP, 64-2-3 for classification of letters (three output neurons, each corresponds to one of the letters).
sample training patterns


## Optimal Architecture?

- For MLP: Too few hidden neurons prevent the network from adequately fitting the data. Too many hidden units can result in overfitting.
(There are advanced methods that prevent overfitting even for rich models, such as regularization, where the error function penalizes overfitting - see PV021.)


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(There are advanced methods that prevent overfitting even for rich models, such as regularization, where the error function penalizes overfitting - see PV021.)
- There are (almost) infinitely many types of architectures of neural networks (convolutional, recurrent, transformers, adversarial, etc.) suitable for various tasks.
- Transfer learning: Start with a known solution to a related problem.

Simplified view: Preserve lower parts of the network trained to solve the related problem (feature extractors). Add your own top part and then train only the new top part (or train the whole network but carefully).

## How to Choose Activation Functions \& Error

- Hidden neurons: "Almost" linear activations such as (leaky)
$\operatorname{ReLU}(y=\max (0, \xi))$
Better than sigmoidal that saturate more often.
- Output neurons: Single output:
- Regression: Typically "linear" output, i.e., no activation on the output neuron.
- Binary classification: Logistic sigmoid $y=1 /\left(1+e^{-\xi}\right)$
- Error: Single output:
- Regression: (Mean) squared error
- Binary classification: Binary cross-entropy

For multiple outputs and classification use softmax output and cross-entropy.

## Applications

- Image recognition, segmentation, etc.
- Machine translation and other text processing
- Text generation, image generation, movie generation, theatre plays generation
- Text to Speech and vice versa
- Finance, business predictions, fraud detection
- Game playing (backgammon is a classical example, AlphaGo is the famous one, computer games are the big ones, bridge is the hard one)
- (artificial brain and intelligence)

Text and image processing are possibly the most advanced deep learning applications.

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- Two layer MLP, $960-4$ - 30 (sometimes $960-5-30$ )


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- Inputs correspond to pixels.
- Sigmoidal activation function (logistic sigmoid).
- Direction corresponds to the center of gravity.
I.e., output neurons are considered as points of mass evenly distributed along a line. Weight of each neuron corresponds to its value.


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Trained while driving.

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- $\vec{x}_{k}=$ image of the road
- $\vec{d}_{k} \approx$ corresponding direction of the steering wheel set by the driver
- the values $\vec{d}_{k}$ computed using Gaussian distribution:

$$
d_{k i}=e^{-D_{i}^{2} / 10}
$$

where $D_{i}$ is the distance between the $i$-th output from the one that corresponds to the real direction of the steering wheel.
(The authors claimed that this approach is better than the binary output because similar road directions induce similar reaction of the driver.)

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- let the driver go crazy! (a bit dangerous, expensive, unreliable)
- Images are very similar (the network basically sees the road from the right lane), overfitting.


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Repetitiveness of images was solved as follows:

- the system has a buffer of 200 images (including the 15 copies of the current one), in every round trains on these images


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- every image of the road has been has been transformed to 15 slightly different copies


Repetitiveness of images was solved as follows:

- the system has a buffer of 200 images (including the 15 copies of the current one), in every round trains on these images
- afterwards, a new image is captured, 15 copies made, and these new 15 substitute 15 selected from the buffer ( 10 with the smallest training error, 5 randomly)


## ALVINN - Training

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The result:

- Training took 5 minutes, the speed was 4 miles per hour (The speed was limited by the hydraulic controller of the steering wheel not the learning algorithm.)
- ALVINN was able to go through roads it never "seen" and in different weather


## ALVINN - Weight Learning

$h 1 \quad h 2 \quad h 3 \quad h 4 \quad h 5$


Here $h 1, \ldots, h 5$ are values of hidden neurons.

## Deep Learning

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- ... but how to train them? The gradient descent suffers from so-called vanishing gradient, intuitively, updates of weights in lower layers are very slow.
- In 2006 a solution was found by Hinton et al:
- Use unsupervised methods to initialize the weights layer by layer so that they capture important features in data. More precisely: The lowest hidden layer learns patterns in data, second lowest learns patterns in data transformed through the first layer, and so on.


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- Use unsupervised methods to initialize the weights layer by layer so that they capture important features in data. More precisely: The lowest hidden layer learns patterns in data, second lowest learns patterns in data transformed through the first layer, and so on.
- Then use a supervised learning algorithm to only fine tune the weights to the desired input-output behavior.
- ... but the true revolution started with convolutional networks trained on several GPUs.


## Convolutional network

A specific architecture of neural networks from 80s.


## Convolutional layers

input neurons


Every neuron is connected with a (typically small) receptive field of neurons in the lower layer.

Neuron is "standard": Computes a weighted sum of its inputs, applies an activation function.

## Convolutional layers



Neurons grouped into feature maps sharing weights.

## Convolutional layers

$28 \times 28$ input neurons
first hidden layer: $3 \times 24 \times 24$ neurons


Each feature map represents a property of the input that is supposed to be spatially invariant.

Typically, we consider several feature maps in a single layer.

## Pooling layers

hidden neurons (output from feature map)


Neurons in the pooling layer compute simple functions of their receptive fields (the fields are typically disjoint):

- Max-pooling : maximum of inputs
- L2-pooling : square root of the sum of squres
- Average-pooling : mean


## Convolutional network



## ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

ImageNet database (16,000,000 color images, 20,000 categories)


## ImageNet Large-Scale Visual Recognition Challenge (ILSVRC)

Competition in classification over a subset of images from ImageNet.

In 2012: Training se 1,200,000 images, 1000 categories. Validation set 50,000, Test set 150,000.

Many images contain several objects $\rightarrow$ typical rule is top- 5 highest probability assigned by the net.

## KSH sít'

ImageNet classification with deep convolutional neural networks, by Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton (2012).


Trained on two GPUs (NVIDIA GeForce GTX 580)
Results:

- Accuracy $84.7 \%$ in top- 5 (second best alg. at the time: 73.8\%)
- $63.3 \%$ in "perfect" classification (top-1)


## ILSVRC 2014

The same set of images as in 2012, top-5 criterium.
GoogLeNet: deep convolutional net, 22 layers


Results:

- $93.33 \%$ in top-5

Superhuman power?

## Superhuman GoogLeNet?!

Andrej Karpathy: ...the task of labeling images with 5 out of 1000 categories quickly turned out to be extremely challenging, even for some friends in the lab who have been working on ILSVRC and its classes for a while. First we thought we would put it up on [Amazon Mechanical Turk]. Then we thought we could recruit paid undergrads. Then I organized a labeling party of intense labeling effort only among the (expert labelers) in our lab. Then I developed a modified interface that used GoogLeNet predictions to prune the number of categories from 1000 to only about 100. It was still too hard - people kept missing categories and getting up to ranges of $13-15 \%$ error rates. In the end I realized that to get anywhere competitively close to GoogLeNet, it was most efficient if I sat down and went through the painfully long training process and the subsequent careful annotation process myself... The labeling happened at a rate of about 1 per minute, but this decreased over time... Some images are easily recognized, while some images (such as those of fine-grained breeds of dogs, birds, or monkeys) can require multiple minutes of concentrated effort. I became very good at identifying breeds of dogs... Based on the sample of images I worked on, the GoogLeNet classification error turned out to be $6.8 \% \ldots$ My own error in the end turned out to be $5.1 \%$, approximately $1.7 \%$ better.

## ILSVRC 2015

- Microsoft network ResNet: 152 layers, complex architecture
- Trained on 8 GPUs
- $96.43 \%$ accuracy in top-5



## ILSVRC



## ILSVRC 2016

Trimps-Soushen (The Third Research Institute of Ministry of Public Security)

There is no new innovative technology or novelty by Trimps-Soushen.

Ensemble of the pre-trained models from previous years.
Each of the models are strong at classifying some categories, but also weak at classifying some categories.
Test error: 2.99\%

## Top-k accuracy analyzed


https://towardsdatascience.com/review-trimps-soushen-winner-in-ilsvrc-2016-image-classificationdfbc423111dd

## Top-20 typical errors

Out of 1458 misclassified images in Top-20:

| Error Categories | Numbers | Percentages(\%) |
| :--- | :---: | :---: |
| Label May Wrong | 221 | 15.16 |
| Multiple Objects (>5) | 118 | 8.09 |
| Non-Obvious Main Object | 355 | 24.35 |
| Confusing Label | 206 | 14.13 |
| Fine-grained Label | 258 | 17.70 |
| Obvious Wrong | 234 | 16.05 |
| Partial Object | 66 | 4.53 |

[^0]
## Top-k accuracy analyzed

Predict:<br>1 pencil box<br>2 diaper<br>3 bib<br>4 purse<br>5 running shoe

Ground Truth:
sleeping bag

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## Top-k accuracy analyzed

## Predict: <br> 1 dock <br> 2 submarine <br> 3 boathouse <br> 4 breakwater <br> 5 lifeboat

Ground Truth: paper towel


## Top-k accuracy analyzed

## Predict:

1 bolete
2 earthstar
3 gyromitra
4 hen of the woods
5 mushroom

## Ground Truth: stinkhorn



## Top-k accuracy analyzed

Predict:<br>1 apron<br>2 plastic bag<br>3 sleeping bag<br>4 umbrella<br>5 bulletproof vest<br>Ground Truth: poncho


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Note that $\frac{\partial E}{\partial w_{j i}}\left(\vec{w}^{(t)}\right)$ is a component of $\nabla E$, i.e. the weight change in the step $t+1$ can be written as follows: $\vec{w}^{(t+1)}=\vec{w}^{(t)}-\varepsilon(t) \cdot \nabla E\left(\vec{w}^{(t)}\right)$.

## MLP - Gradient Computation

For every weight $w_{j i}$ we have (obviously)

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\frac{\partial E}{\partial w_{j i}}=\sum_{k=1}^{p} \frac{\partial E_{k}}{\partial w_{j i}}
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Applying the chain rule we obtain

$$
\frac{\partial E_{k}}{\partial w_{j i}}=\frac{\partial E_{k}}{\partial y_{j}} \cdot \sigma_{j}^{\prime}\left(\xi_{j}\right) \cdot y_{i}
$$

where (more applications of the chain rule)

$$
\begin{aligned}
& \frac{\partial E_{k}}{\partial y_{j}} \text { is computed directly for the output neurons } j \in Y \\
& \frac{\partial E_{k}}{\partial y_{j}}=\sum_{r \in j \rightarrow} \frac{\partial E_{k}}{\partial y_{r}} \cdot \sigma_{r}^{\prime}\left(\xi_{r}\right) \cdot w_{r j} \quad \text { for } j \in Z \backslash(Y \cup X)
\end{aligned}
$$

(Here $y_{r}=y[\vec{w}]\left(\vec{x}_{k}\right)$ where $\vec{w}$ are the current weights and $\vec{x}_{k}$ is the input of the $k$-th training example.)

## Multilayer Perceptron - Backpropagation

Input: A training set $D=\left\{\left(\vec{x}_{k}, \vec{d}_{k}\right) \quad \mid k=1, \ldots, p\right\}$ and the current vector of weights $\vec{w}$.
Note that the backprop. is repeated in every iteration of the gradient descent!

- Evaluate all values $y_{i}$ of neurons using the standard bottom-up procedure with the input $\vec{x}_{k}$.


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- Evaluate all values $y_{i}$ of neurons using the standard bottom-up procedure with the input $\vec{x}_{k}$.
- For every training example $\left(\vec{x}_{k}, \vec{d}_{k}\right)$ compute $\frac{\partial E_{k}}{\partial y_{j}}$ using backpropagation through layers top-down :
- For all $j \in Y$ compute $\frac{\partial E_{k}}{\partial y_{j}}$ by taking the derivative of the error.
e.g., in the case of the squared error we have $\frac{\partial E_{k}}{\partial y_{j}}=y_{j}-d_{k j}$.


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- In the layer $\ell$, assuming that $\frac{\partial E_{k}}{\partial y_{r}}$ has been computed for all neurons $r$ in the layer $\ell+1$, compute

$$
\frac{\partial E_{k}}{\partial y_{j}}=\sum_{r \in j \rightarrow} \frac{\partial E_{k}}{\partial y_{j}} \cdot \sigma_{r}^{\prime}\left(\xi_{r}\right) \cdot w_{r j}
$$

for all $j$ from the $\ell$-th layer. Here $\sigma_{r}^{\prime}$ is the derivative of $\sigma_{r}$.

- Put $\frac{\partial E_{k}}{\partial w_{j i}}=\frac{\partial E_{k}}{\partial y_{j}} \cdot \sigma_{j}^{\prime}\left(\xi_{j}\right) \cdot y_{i}$

Output: $\frac{\partial E}{\partial w_{j i}}=\sum_{k=1}^{p} \frac{\partial E_{k}}{\partial w_{j i}}$.


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